REPORT
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Investigation of   Receiver Techniques and Detectors for Use at
Millimeter and Submillimeter Wave Lenghts

Subject of Report   Annual Summary Report
1 October 1966 to 30 September 1967

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ANNUAL SUMMARY REPORT
1 October 1966 to 30 September 1967

INTRODUCTION

The research activity concerning the first part of the period was presented in the semiannual status report of May 1967.[1] If suffices here to outline only some of the points given there. On the theoretical side we had started to calculate the excitation cross-sections for some of the vibrational energy levels of CO_2 colliding with He and also finding some of the CO_2 force constants. Meanwhile, we had found that burning hydrocarbons in a discharge would give us by-products such as CO, CO_2[2] and possibly a number of other intermediate by-products of free radicals. However, the resulting radiation from this discharge always ended in the CO_2 and CO laser lines. Considerable time was spent in measuring and determining the spectral output. It was found that the bulk of coherent radiation was in the 10.6 or 9.6 micron region characteristic of CO_2 or the 5 micron region characteristic of the CO vibrational levels.

SUMMARY OF THE WORK DONE OR COMPLETED WITHIN THE LAST SIX MONTHS

a. Two different species of freon[3] gas were made to lase with the addition of helium gas. The spectral output of this gas was found to be in the near infrared region of the spectrum. About nine new lines were found. Theoretical investigation to determine the assignments of the laser lines was not fruitful.

b. In the argon II, neon II and krypton II gas lasers it has been assumed that the gas is ionized from the long lived metastable states[4] (since it takes only a few electron volts to ionize it), rather than from the ground state. The question asked was: when the metastable electron is removed, is it possible to have at the same time an electron shaken off to give an excited state to the ion? Calculations to determine this possibility were performed and cross sections were calculated for the three gases in question. The calculations showed that such a situation was, in fact, quite possible.[5]

c. The transition probabilities as well as the life times of some of the $2p^4$-3p excited states of NeII and $4p^4$-5p excited states of KrII were

calculated by determining experimentally the radial integrals F_n and G_n and applying the computer program first developed for the CO_2 eigen states.[1] Later, the radial integrals were calculated directly by first finding the radial wave functions and then directly integrating the functions. The two methods, checked quite well and the life times found are reasonable.

d. Because of the close proximity of some of the vibrational levels of arsine with that of $N_2(\nu=1)$ vibrational level,[6] the vibrational rotational spectrum of AsH_3, in the 5-μ region, was partially analysed. Difficulties arose from the fact that the three possible bands, namely $2\nu_1$, $2\nu_3$ and $\nu_1 + \nu_3$, lie close to one another and a number of possible interactions such as Fermi resonance can alter the position of the band center. The two strong bands are assigned as $2\nu_1$ and $2\nu_3$. Vibrational-rotational molecular constants as well as band centers have been obtained.

e. Having derived the degree of mixing of the excited levels of the NeII $2p^4$-3p level, as well as the $4p^4$-5p levels of KrII, the direct excitation cross sections to those levels were calculated by using the method of sudden perturbation[7] as discussed in a previous report.[8] These results showed that because of the greater degree of mixing of the states of KrII, the direct excitation cross section value is evenly distributed among all levels with the total angular momentum quantum number $J = 3/2$ and $J = 1/2$.

PROPOSED FUTURE PROGRAM
OCTOBER 1967 TO SEPTEMBER 1968

A. Introduction

For the coming year, we are interested in continuing our calculations on the effect of the collision of simple gases with the CO_2 molecule. It has been shown[1] that when foreign gases such as N_2, He, H_2O or H_2 are introduced into a CO_2 discharge, the lifetime of certain vibrational levels changes drastically. This in turn could effect the intensity distribution of the emanated infrared. The purpose of this work is to study theoretically the de-excitation cross section of some of the CO_2 vibrational levels by collision.

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B. Method of Calculation

When a vibrationally excited molecule within a discharge tube makes a collision with another molecule or atom, depending upon the temperature of the gas, the vibrational energy of the first molecule can be transferred to the kinetic energy of the second molecule or atom. However, if the second molecule has a vibrational energy, or a harmonic of that energy, close to the vibrational energy of the first, then it is possible for the first molecule to vibrationally excite the second molecule. It is the purpose of this work to calculate the cross section for the transfer of vibrational energy from one simple molecule to the kinetic or vibrational energy of another simple molecule. In particular, we are interested in the interaction of the CO_2 molecule with other molecules such as H_2, He, N_2 and CO_2. In works available[3] on the calculation of the excitation cross section of vibrational to kinetic energy transfer in CO_2 performed by other researchers, it has mostly been assumed for the sake of simplification that the vibrational levels of the CO_2 molecule are pure states and calculations have been done with this assumption in mind. However, due to the anharmonicity of the potential function and the existence of the Fermi-resonances between the various vibrational levels, the states do not remain pure, but are rather mixed. This consideration can give different results for the cross sections. The Hamiltonian for the CO_2 molecule, up to the quartic anharmonic terms, has been given[2] and the force constants are fairly accurately determined. For this reason one can determine the degree of the mixing of the wave functions. Already we have diagonalized matrices up to 48 by 48 using force constants given by Denison (1940)[9] and also force constants calculated from more recent observations. The Hamiltonian for the CO_2 molecule is given by

$$(1) \qquad H_{vib}(CO_2) = \frac{2\pi^2 c}{h} \left[\omega_1 p_\sigma^2 + \omega_2 (p_\xi^2 + p_\eta^2) + \omega_3 p_\zeta^2 \right]$$

$$+ \frac{1}{2} hc(\omega_1 \sigma^2 + \omega_2 \rho^2 + \omega_3 \zeta^2) + hc(a\sigma^3 + b\sigma\rho^2 + c\sigma\zeta^2)$$

$$+ hc(d\sigma^4 + e\rho^4 + f\zeta^4 + g\sigma^2\rho^2 + h\sigma^2\delta^2 + i\rho^2\zeta^2)$$

where ξ, σ, η and ζ are the normal coordinates given by the following relations

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(2)
$$\sigma = 2\pi(\omega_1 m c_o/2h)^{\frac{1}{2}}q \quad \eta = 2\pi(\omega_2 \mu c_o/h)^{\frac{1}{2}}y, \quad \rho^2 = \xi^2 + \eta^2$$

$$\xi = 2\pi(\omega_2 \mu c_o/h)^{\frac{1}{2}}x \quad \zeta = 2\pi(\omega_3 \mu c_o/h)^{\frac{1}{2}}z$$

m is the mass of oxygen and $\mu = 2mM/2m+M$ is the reduced mass with M the mass of carbon, q measures the change in distance between the two oxygen atoms and x, y, z are the coordinates of the carbon atom with respect to the center of gravity of the two oxygen atoms, with the z axis oriented along q. Finally, a, b, c...etc. are the anharmonic force constants. When the CO_2 molecule makes a collision with another atom or molecule such that there is a transfer of energy between the vibrational energy of CO_2 and the kinetic energy of the colliding particle, the Hamiltonian for such a process is written in the following form

(3)
$$= H_{vib}(\sigma\rho\zeta) + H_{interaction}(r, \sigma, \rho, \zeta) + H_{kinetic}(r)$$

where $H_{kinetic}$ is simply the kinetic energy of the incoming particle compared to a frame of reference in which CO_2 is at rest. The interaction potential is however not easily determinable, but can be approximately written in the form of

(4)
$$V_{int.} = V(r) V(\sigma) V(\rho) V(\zeta)$$

where it has been assumed that the potential is separable. However, it should be kept in mind that this is an approximation. $V(r)$ is usually taken to be Leonard-Jones potential and for ease of calculation and because of the short range effect of the interaction potentials $V(\sigma)$, $V(\rho)$, or $V(\zeta)$ are assumed to have an exponential form of the type $e^{-A\sigma}$ where A is determined usually by matching the exponential to a Leonard-Jones potential at the point of the classical nearest approach.

When there is a vibrational exchange of energy between two molecules another term has to be added to the Hamiltonian of Eq. (3) which corresponds to the vibrations of the second molecule and moreover the intereaction potential has to be modified. Some detailed work on this subject has been given by Takayanagi[10] with an extensive bibliography.[11]

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